TABLE I. Supplement: Coordinates[a] for the atoms in compound **9**

atom	x	y	z
C	4.8230510044	-0.3202431448	-0.6322330717
C	5.3314123096	-0.8463867416	0.7170130084
N	6.5107271908	-1.6855480060	0.6318883857
H	4.6138234392	-1.1427535941	-1.3057447175
H	5.6064503504	0.2643353318	-1.1045595255
H	5.5606951848	-0.0027495506	1.3609009242
H	4.5491144263	-1.4070772611	1.2146705592
H	6.3362950750	-2.5151741063	0.0985787343
H	7.2773984780	-1.2046072295	0.2026040968
O	-1.9488737966	-2.4437315046	0.1652261903
O	-3.3598489565	1.8117499560	0.5132628936
N	-2.6570397602	-0.3207840034	0.3942461687
C	-0.2950912589	-0.7895881805	-0.0172085241
C	0.7249681017	-1.6785108577	-0.2103238109
C	2.0460594129	-1.2521944717	-0.3801761210
C	2.3705111016	0.0893216663	-0.3718209382
C	1.5197001319	2.4557073435	-0.2514894690
C	0.4931876216	3.3381757890	-0.0827623759
C	-0.8125820052	2.8660455104	0.1317642030
C	-1.0568719225	1.5227681644	0.1593240834
C	-0.0064679805	0.5936380213	-0.0177017292
C	1.3100764817	1.0560048559	-0.2094190026
C	-1.6698280683	-1.2769089962	0.1799013630
C	-2.4484710511	1.0462778508	0.3686119263
H	-1.6292561986	3.5488702926	0.2656579527

H	0.5023513057	-2.7286330004	-0.2159769515
H	2.8090459642	-1.9943427421	-0.5023698772
H	0.6786821099	4.3954831305	-0.1231013306
H	2.4985591246	2.8528974317	-0.4429622112
N	3.6549490042	0.5319047787	-0.5454213400
H	3.8443303750	1.4547608002	-0.2347824217
N	-6.1703655159	-1.4182275536	-0.5187698382
C	-4.8084709850	-0.9487928752	-0.6943895358
C	-4.0287500243	-0.7959085467	0.6132451245
H	-6.1890681707	-2.3165983394	-0.0755749081
H	-6.6998123881	-0.7879283107	0.0524242232
H	-4.8410956121	0.0062437193	-1.2054662598
H	-4.2886909644	-1.6462343143	-1.3405213356
H	-3.9633445889	-1.7447905237	1.1217432384
H	-4.5181895358	-0.0836981790	1.2589527244
F^{-1}	-3.2987456322	-2.4458334126	0.2186043721

[a] In units of Å.